

TABLE OF CONTENTS

CHAPTER	TITLE	PAGE
	THESIS STATUS	
	SUPERVISOR'S DECLARATION	
	TITLE PAGE	i
	DECLARATION PAGE	ii
	DEDICATION	iii
	ACKNOWLEDGEMENTS	iv
	ABSTRACT	v
	ABSTRAK	vi
	TABLE OF CONTENTS	vii
	LIST OF TABLES	xi
	LIST OF FIGURES	xii
	LIST OF SYMBOLS	xiv
	LIST OF APPENDICES	xvi
I	INTRODUCTION	1
	1.1 Background Information	1
	1.2 Problem Statement	4
	1.3 Objective and Scopes of Study	4
	1.3.1 Development of Base Case Simulation	5

1.3.2	Base Case Model Validation	5
1.3.3	Autothermal Reactor (ATR) Optimization	5
1.3.4	Heat Integration	6
1.3.5	Carbon Monoxide (CO) Clean Up	6
1.3.6	Plant Wide Optimization	7
1.4	Thesis Organization	8
II	LITERATURE REVIEW	9
2.1	Hydrogen Production for Fuel Cell	9
2.2	Hydrogen Production from Jet Fuel	12
2.2.1	Steam Reforming of Jet Fuel	15
2.2.2	Partial Oxidation of Jet Fuel	16
2.2.3	Autothermal Reforming of Jet Fuel	16
2.3	Hydrogen Production from Jet Fuel via Catalytic Auto thermal Reforming	17
2.4	Simulation and Optimization of Hydrogen Production Plant from Jet Fuel	19
2.5	Summary	19
III	METHODOLOGY	21
3.1	Research Tools	21
3.1.1	Aspen HYSYS 2004.1	21
3.2	Research Activities	22
3.2.1	Data Collection	23
3.2.2	Steady State Model Development	26
3.2.3	Steady State Model Validation	26
3.2.4	Optimization of Developed Model	26
3.3	Summary	27
IV	SIMULATION AND OPTIMIZATION OF HYDROGEN PRODUCTION PLANT FOR FUEL CELL APPLICATIONS	28
4.1	Process Description of Hydrogen Production	

	from Jet fuel	28
4.2	Modelling and Simulation of Hydrogen	
	Production from Jet Fuel Cell	29
4.2.1	Physical Properties	31
4.2.2	Thermodynamic Properties	31
4.2.3	Integration Algorithm	33
4.3	Summary	34
V	RESULTS AND DISCUSSION	35
5.1	Base Case Simulation	36
5.1.1	The ATR Reactor	38
5.2	Base Case Model Validation	40
5.3	Autothermal Reactor (ATR) Optimization	41
5.4	Heat Integration System	43
5.5	Carbon Monoxide (CO) Clean Up	44
5.5.1	Water Gas Shift (WGS)	45
5.5.2	Preferential Oxidation (PROX)	48
5.6	Plant Wide Optimization	50
5.6.1	Water Gas Shift (WGS)	51
5.6.2	Preferential Oxidation (PROX)	53
5.7	Plant Wide Analysis	55
5.7.1	Temperature Profile	55
5.7.2	Efficiency of the Fuel Processor	56
5.8	Summary	57
VI	CONCLUSIONS AND RECOMMENDATIONS	58
6.1	Summary	58
6.2	Conclusions	59
6.3	Recommendations	60
6.3.1	Purification of Hydrogen	60

6.3.2	Water Management	60
6.3.3	Dynamic Analysis	61
REFERENCES		62
Appendices A - C		68

LIST OF TABLES

TABLE NO.	TITLE	PAGE
3.1	Lower heating values	23
3.2	Gas composition in autothermal reforming of jet fuel (GHSV = 50,000h ⁻¹ , S/C = 1.5, P = 1 bar)	25
4.1	Physical properties of the components	31
5.1	Effluent of ATR reactor	39
5.2	Comparison between calculation result and simulation result	40
5.3	Comparison between before and after optimization at ATR reactor	43
5.4	Composition of components after ATR and WGS reactors	47
5.5	Composition of components after LTS and after PROX At 0 kgmole/h inject air	50
5.6	Comparison of components between before and after optimization at PROX reactor	54

LIST OF FIGURES

FIGURE NO.	TITLE	PAGE
3.1	PFD of the laboratory test rig	24
3.2	Process flow of the hydrogen plant development	27
4.1	Schematic illustration of the hydrogen production process	29
4.2	HYSYS Simulation Environment	30
4.3	Simulation stages using Aspen HYSYS 2004.1	34
5.1	PFD of the ATR reactor	38
5.2	Production of H ₂ and CO versus molar flow of air	42
5.3	Temperature [°C] at ATR versus air molar flow	42
5.4	The heat integration system	44
5.5	Carbon monoxide clean-up using water gas shift process	46
5.6	Carbon monoxide clean-up using water gas shift and preferential oxidation system	49
5.7	Production of H ₂ and CO at LTS versus molar flow of water	51
5.8	Temperature after HX3 and before HTS versus molar flow of water	52
5.9	Composition of CO [ppm] versus inject air at PROX	53

5.10	Temperature profile of the hydrogen production plant	55
5.11	Hydrogen and CO profile	57

LIST OF SYMBOLS

λ	-	Air to fuel ratio
Al	-	Aluminium
ANL	-	Argonne National Laboratory
ATR	-	Autothermal Reforming
C	-	Carbon
CO ₂	-	Carbon Dioxide
CO	-	Carbon Monoxide
CSTR	-	Continuously Stirred Tank Reactor
°C	-	degree Celcius
ft ³	-	cubic feet
g/L	-	gram per litre
gmol ⁻¹	-	gram per mol
GHSV	-	Gas Hourly Space Velocity
h	-	hour
H	-	Hydrogen(atom)
HCs	-	Hydrocarbons
H ₂	-	Hydrogen(molecule)
H ₂ O	-	Water
K	-	Kelvin
kJ mol ⁻¹	-	kilo Joule per mol
kW	-	kilo Watt
LHSV	-	Liquid Hourly Space Velocity
LHV	-	Lower Heating Value
mol/h	-	mol per hour
m ³	-	cubic meter

m^3/h	-	cubic meter per hour
Ni	-	Nickel
O_2	-	Oxygen(molecule)
ODE	-	Ordinary Differential Equation
P	-	Pressure
PEMFC	-	Proton Exchange Membrane Fuel Cell
POX	-	Partial Oxidation
PROX	-	Preferential Oxidation
Ru	-	Ruthenium
RXNEQ	-	a thermodynamics equilibrium computer code developed by Haynes(1990)
S/C	-	Steam to carbon ratio
Si	-	Silica
SR	-	Steam-Reforming
STP	-	standard temperature and pressure [298.15 K and 101.325 kPa (1 atm)]
TOX	-	Total Oxidation
w	-	work
WGS	-	Water Gas Shift

LIST OF APPENDICES

APP. NO.	TITLE	PAGE
A	Results of every stream in the hydrogen production plant for fuel cell applications	69
B	Patterns of composition of all components at every reactor	72
C	Calculation scheme of efficiency of the fuel processor	73